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TURBULENT CONVECTION WITH OVERSHOOTING: REYNOLDS STRESS APPROACH

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ABSTRACT

Turbulent convection is a phenomenon relevant to both stellar structure and accretion disks. In the latter, a basic parameter such as the turbulent viscosity ν_t is still treated phenomenologically; in the case of stellar structure, most of the work still relies on the mixing-length theory (MLT) which assumes homogeneity and thus lacks *diffusion terms* (divergence of third-order moments like $\overline{w^2\theta}$, $\overline{w\theta^2}$, $\overline{q^2w}$). To include them, one needs a new formalism. We review and discuss the Reynolds stress approach (proven successful in other fields) which provides a set of coupled differential equations that yield all the turbulent quantities of interest. Although the system can only be solved numerically, some features can be listed:

1. The convective flux $F_c = c_p \rho \overline{w\theta}$ is not given simply by (κ_t is the turbulent conductivity)

$$F_c = F_c^{\rm MLT} \approx \kappa_t(\nabla - \nabla_{\rm ad}) .$$

2. Inclusion of the diffusion terms related to $\overline{w^2\theta}$ and $\overline{w\theta^2}$ contributes a *countergradient* term Γ_c, which may *carry heat from cold to hot regions,*

$$F_c \approx \kappa_t(\nabla - \nabla_{\rm ad} + \Gamma_c) .$$

The term Γ_c was first discussed by Deardorff in the context of atmospheric turbulence.

3. Inclusion of the diffusion term related to $\frac{1}{2}\overline{q^2 w}$ (turbulent kinetic energy flux) contributes an additional term (first discussed in atmospheric turbulence by Tennekes)

$$F_c \approx \kappa_t(\nabla - \nabla_{\rm ad} + \Gamma_c) + F_c^{\rm diff} ,$$

which is responsible for *overshooting.*

In addition to the convective flux, we also derive a model expression for ν_t as a function of both shear and buoyency: it is needed in the numerical simulation of stellar convection and in accretion disks to replace the phenomenological expressions used thus far.

Subject headings: accretion, accretion disks — convection — stars: interiors — turbulence

1. INTRODUCTION

The complexity of turbulence is such that we do not yet possess a general theory to describe different types of turbulent flows. For reasons based more on practical considerations than on a priori choices, more attention has been devoted in the past to turbulence generated by mean velocity gradients than mean temperature gradients, that is, turbulent convection, which is, however, a phenomenon of great relevance to studies of stellar structure and accretion disks. In the latter, turbulent convection is still treated with mixing-length theory (MLT), whereas modern turbulence theories permit a significantly more accurate treatment. In that spirit, Canuto & Mazzitelli (1991, hereafter CM1) recently employed a successful model of homogeneous turbulence—the EDQNM model (Eddy-Damped Quasi-Normal Markovian: Orzsag 1977; Lesieur 1990)—to compute the convective flux appropriate to a stellar interior. The new treatment incorporated, among other things, the contribution of eddies of all sizes, thereby overcoming the rather extreme MLT assumption that the full eddy spectrum can be represented by one large eddy. The new model (CM1; Canuto & Mazzitelli 1992, hereafter CM2) has interesting astrophysical consequences.

However, the original EDQNM model and even the more complete DIA model (Direct Interaction Approximation: Kraichnan 1964) have limitations: they can only describe *homogeneous turbulence.* As the onset of turbulence of almost any kind is known to entail strong mixing and smoothing of large gradients in both mean quantities (e.g., the temperature) and second-order correlations (e.g., the convective flux $\overline{w\theta}$, turbulent energies $\overline{w^2}$, etc., where w and θ are the turbulent or fluctuating velocity and temperature), one may be tempted to conclude that the homogeneity approximation is fairly safe. This is conditionally true, as experiments by Willis & Deardorff (1974) have demonstrated: the core of a convective zone is indeed nearly homogeneous, but large gradients and, thus, inhomogeneities occur in regions comprising approximately 10% of the thickness of the convective region. Accordingly, when only bulk properties are required, the homogeneity approximation may be reasonable, but as soon as phenomena occurring in the vicinity of the transition region need to be described, a more complete formalism able to incorporate inhomogeneities must be employed.

In the context of stellar convection, a conspicuous manifestation of inhomogeneity is "overshooting," a phenomenon that has a long and somewhat controversial history: see Marcus et al. (1983), Zahn (1991), Andersen, Nordstrom, & Clausen et al. (1990), VandenBerg & Poll (1989), and Stothers & Chin (1991). The contradictory results that have appeared in the literature over the past 25 years should not be viewed as casting doubt on the existence of the phenomenon which geophysical and laboratory experiments have confirmed; rather, they are a reflection of the inadequacy of the MLT. The problem is that MLT and overshooting do not mix. MLT treats turbulence as homogeneous, whereas overshooting is a distinctive feature of the inhomogeneous nature of convection in the transition region. Thus, while the MLT has proven to be a useful tool to estimate bulk properties which are possibly less sensitive to whether homogeneity is assumed or not, it cannot incorporate overshooting.

In this paper we adopt the Reynolds stress formalism to treat turbulent convection: the formalism has a rather long history, and it has been successfully applied to laboratory and atmospheric turbulence (Zeman 1981; Speziale 1991). It is the goal of this paper to review this methodology and suggest that it may prove very useful to treat stellar and accretion disk turbulent convection, as well as in the construction of the subgrid models needed in large eddy simulations (Chan & Sofia 1989; Hossain & Mullan 1991). The final result consists of a set of differential equations that yield the mean and turbulent quantities, such as convective fluxes, turbulent viscosity, turbulent conductivity, etc.

2. THE PROBLEM

Let θ and w be the turbulent temperature and velocity (in the z-direction). The definition of the convective flux F_c is then (an overbar means ensemble average)

$$F_c = c_p \rho \overline{w\theta} , \tag{1}$$

and the goal is to express $\overline{w\theta}$ as a function of the Rayleigh number

$$\mathrm{Ra} \equiv \frac{g\alpha\beta\ell^4}{\nu\chi} , \tag{2}$$

where g is the local gravity, α is the thermal expansion coefficient, ℓ is a mixing length, and β is the overadiabatic gradient, $(\partial T/\partial z)_{\mathrm{ad}} = -g/c_p$,

$$\beta = -\left[\frac{\partial T}{\partial z} - \left(\frac{\partial T}{\partial z}\right)_{\mathrm{ad}}\right] = TH_p^{-1}(\nabla - \nabla_{\mathrm{ad}}) . \tag{3}$$

Moreover, $\chi \equiv K/c_p\rho$ is the thermometric conductivity, while K is the thermal conductivity; finally, ν is the kinematic viscosity. Since in stellar interiors ν is exceedingly small compared to χ (for the Sun, the Prandtl number $\sigma = \nu/\chi \approx 10^{-9}$; Massaguer 1990), it is more convenient to use a variable independent of viscosity, that is, the product

$$\sigma\,\mathrm{Ra} \equiv S = \frac{g\alpha\beta\ell^4}{\chi^2} . \tag{4}$$

In astrophysical notation,

$$S = 162A^2(\nabla - \nabla_{\mathrm{ad}}) , \tag{5}$$

$$A = \frac{c_p\rho^2\kappa\ell^2}{12acT^3}\left(\frac{g}{2H_p}\right)^{1/2} \tag{6}$$

(Cox & Giuli 1968), where κ is the opacity and the remaining symbols have their usual meaning. Since the radiative flux F_r has the form

$$F_r = -K\frac{\partial T}{\partial z} , \tag{7}$$

the MLT suggests writing equation (1) so as to exhibit the structure (7), that is,

$$F_c^{\mathrm{MLT}} = -K_t\left[\frac{\partial T}{\partial z} - \left(\frac{\partial T}{\partial z}\right)_{\mathrm{ad}}\right] , \tag{8}$$

where K_t is a turbulent or eddy conductivity for which the MLT suggests the expression

$$K_t/c_p\rho = \kappa_t \approx \bar{q}\ell , \tag{9}$$

where $\frac{1}{2}\overline{q^2}$ is the turbulent kinetic energy. Thus, the basic MLT formula for the convective flux becomes (Böhm-Vitense 1958; Cox & Giuli 1968; Spruit, Nordlund, & Title 1990)

$$F_c = c_p\rho\beta\chi\Phi , \tag{10}$$

$$\Phi = \kappa_t/\chi , \tag{11}$$

and the problem then reduces to that of finding the dimensionless function Φ versus S. If one assumes that the heat transport by the eddies occurs without losses due to radiative processes, equation (10) should be independent of χ. Since $S \sim \chi^2$, this demands that

$$\Phi \propto S^{1/2} \sim \beta^{1/2}\ell^2\chi^{-1} , \tag{12}$$

yielding the well-known result (Schwarzschild 1958)

$$F_c \sim (\nabla - \nabla_{\mathrm{ad}})^{3/2}\ell^2 . \tag{13}$$

When heat losses by the traveling eddies (Öpik 1950) are accumulated for, the new formula for Φ is (Cox & Giuli 1968; Gough & Weiss 1976; Canuto & Goldman 1985)

$$\Phi = S^{-1}[(1+S)^{1/2}-1]^3 , \tag{14}$$

which reduces to $S^{1/2}$ in the case of large convective efficiency $\Gamma = (S+1)^{1/2} - 1$.

CM1 have recently pointed out that the inviscid nature of stellar interiors renders the basic MLT tenet (the dominance of one large eddy) a singularly poor approximation. In fact, in any turbulent flow, the lower the viscosity, the wider is the range (spectrum) of eddies that characterize it. Specifically, the ratio between the largest L and the smallest ℓ_0 eddies can be shown to be $L/\ell_0 \sim \nu^{-3/4} \sim \sigma^{-3/4}$. As shown in Figure 1 of CM1, for a Prandtl number of $\sigma \simeq 10^{-3}$, the ratio is about 10^6. As discussed in CM1, the evaluation of the full turbulent energy spectrum requires the use of a turbulence model, and CM1 adopted the EDQNM model (Orszag 1977; Lesieur 1990). Once full the eddy spectrum is obtained, the convective flux F_c can be computed. As expected, the larger number of eddies leads to a larger flux. As shown in CM, for large convective efficiencies, the new flux is $F_c \approx 10F_c^{\mathrm{MLT}}$, in agreement with the numerical simulation of convective turbulence by Cabot et al. (1990).

3. THE FUNDAMENTAL EQUATIONS

The Navier-Stokes equations for the total velocity field v_i are given by

$$\tilde{\rho}\left(\frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j}\right)v_i = -\tilde{p}_{,i} - \tilde{\rho} g_i + \mu v_{i,jj} - 2\tilde{\rho}\epsilon_{ijk}\Omega_j v_k , \tag{15}$$

where $a_{,i} = \partial a/\partial x_i$, $\tilde{\rho}$ and $\tilde{p}$ are the total density and pressure, $g_i = (0, 0, g)$, $\mu/\tilde{\rho} = \nu$ is the kinematic viscosity, ϵ_{ijk} is the antisymmetric tensor, and $\mathbf{\Omega}$ is the angular velocity vector. Let us now write

$$\tilde{p} = p_0 + P_* , \qquad \tilde{T} = T_0 + T_* , \qquad \tilde{\rho} = \rho_0 + \rho_* , \tag{16}$$

where the static components p_0 and ρ_0 satisfy the hydrostatic equilibrium equation

$$\frac{\partial p_0}{\partial x_i} = -\rho_0 g_i . \tag{17}$$

The remaining P_*, T_*, and ρ_* correspond to the parts affected by the motion, that is, by the velocity field: since the latter has an average and a fluctuating (or turbulent) part, they will be further split in the two corresponding components (see eq. [28]). For the time being, substituting equations (16) and (17) into equation (15), we obtain

$$\left(\frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j}\right)v_i = -\frac{1}{\tilde{\rho}} P_{*,i} - \left(1 - \frac{\rho_0}{\tilde{\rho}}\right)g_i + \nu v_{i,jj} - 2\epsilon_{ijk}\Omega_j v_k . \tag{18}$$

Let us consider the coefficient of g_i. Using the equation of state for a perfect gas

$$\tilde{p} = R\tilde{\rho}\tilde{T} , \qquad p_0 = R\rho_0 T_0 , \tag{19}$$

we derive the relation

$$1 - \frac{\rho_0}{\tilde{\rho}} = \left(1 + \frac{P_*}{p_0}\right)^{-1}\left(\frac{P_*}{p_0} - \frac{T_*}{T_0}\right). \tag{20}$$

Since we cannot treat the case of fully compressible turbulence (represented here by the term P_*/p_0), but at the same time we want to account for some of its effects, we shall write equation (20) as

$$1 - \frac{\rho_0}{\tilde{\rho}} = -\frac{T_*}{T_0} + \frac{P_*}{p_0} + O\left[\left(\frac{P_*}{p_0}\right)^2, \left(\frac{T_*}{T_0}\right)\left(\frac{P_*}{p_0}\right)\right], \tag{21a}$$

which, within the Boussinesq approximation, further simplifies to

$$1 - \frac{\rho_0}{\tilde{\rho}} = -\alpha T_* , \tag{21b}$$

where α is the thermal expansion coefficient T_0^{-1}. Inserting equation (21b) into equation (18), we obtain

$$\left(\frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j}\right)v_i = -P_{*,i} + \lambda_i T_* + \nu v_{i,jj} - 2\epsilon_{ijk}\Omega_j v_k , \tag{22}$$

where $\lambda_i = g_i \alpha$. For ease of notation, the density ρ_0 is taken to be unity.

Next, consider the temperature field. For that, we begin with the equation for the entropy Σ,

$$\tilde{\rho}\tilde{T}\left(\frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j}\right)\Sigma = -F^r_{i,i} + Q , \tag{23}$$

$$F_i^r = -K \frac{\partial \tilde{T}}{\partial x_i} . \tag{24}$$

F_i^r is the radiative flux, and Q represents an external source of energy. Using the definition

$$\tilde{T} d\Sigma = c_p d\tilde{T} - \tilde{\rho}^{-1} d\tilde{p} \tag{25}$$

as well as equations (16) and (17), we derive (the hydrostatic variables are time independent) the equation satisfied by the temperature T_*, that is,

$$\left(\frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j}\right) T_* = \beta_j^0 v_j + (c_p \rho_0)^{-1}\left(\frac{\partial}{\partial t} + v_j \frac{\partial}{\partial x_j}\right) P_* + \chi \frac{\partial^2 T_*}{\partial x_j^2} , \tag{26}$$

where

$$\beta_j^0 \equiv -\left(\frac{\partial T_0}{\partial x_j} + \frac{g_j}{c_p}\right) , \tag{27a}$$

$$Q \equiv F_{i,i}^r(T_0) . \tag{27b}$$

In atmospheric turbulence, equation (26) coincides with equation (2.19) of Donaldson (1973) who also assumes $\beta_j^0 = 0$, corresponding to an isentropic basic state, and who neglects the P_* term since it is of second order in the Mach number. In stellar convection, equation (34) of Spiegel & Veronis (1960) is equivalent to equation (26) without the pressure term P_*.

Equations (22) and (26) are our basic set of equations. Next, we split each field into its average and fluctuating parts, that is, we write

$$v_i = U_i + u_i , \qquad P_* = \Pi + p , \qquad T_* = \Theta + \theta , \tag{28}$$

where the fluctuating or turbulent components have zero average, $\bar{u}_i = 0$, $\bar{p} = 0$, and $\bar{\theta} = 0$. In the case of the pressure and temperature fields, since there is a static component, the physical average field is

$$\bar{\tilde{T}} = T_0 + \Theta \equiv T , \qquad \bar{\tilde{p}} = p_0 + \Pi \equiv P , \tag{29}$$

that is, the symbols T and P will be used for the true average temperature and pressure. Substitute equation (28) into equations (22) and (26), average the resulting expressions, and subtract the latter from the full equations. The result is

$$\frac{DU_i}{Dt} = -\frac{\partial \Pi}{\partial x_i} + \lambda_i \Theta - \frac{\partial}{\partial x_j} \overline{u_i u_j} + \nu \frac{\partial^2 U_i}{\partial x_j^2} - 2\epsilon_{ijk} \Omega_j U_k , \tag{30}$$

$$\frac{Du_i}{Dt} = -\frac{\partial p}{\partial x_i} - u_j \frac{\partial U_i}{\partial x_j} - \frac{\partial}{\partial x_j} (u_i u_j - \overline{u_i u_j}) + \lambda_i \theta + \nu \frac{\partial^2 u_i}{\partial x_j^2} - 2\epsilon_{ijk} \Omega_j u_k , \tag{31}$$

$$\frac{D\Theta}{Dt} = \beta_j^0 U_j + \chi \frac{\partial^2 \Theta}{\partial x_j^2} - \frac{\partial}{\partial x_j} \overline{u_j \theta} , \tag{32a}$$

$$\frac{D\theta}{Dt} = -u_j\left(\frac{\partial T}{\partial x_j} + \frac{g_j}{c_p}\right) - \frac{\partial}{\partial x_j} (u_j \theta - \overline{u_j \theta}) + \chi \frac{\partial^2 \theta}{\partial x_j^2} , \tag{32b}$$

where $D/Dt = \partial/\partial t + U_j \partial/\partial x_j$.

In the case of static convection without a mean flow, the left-hand side of equation (32a) vanishes. Integrate once using a plane geometry (eqs. [7] and [27b]). If we call $F_{\rm ext}$ the integral of Q, we obtain the *flux conservation law* valid at any level z,

$$F_r(z) + F_c(z) = F_{\rm ext}(z) . \tag{33}$$

4. SECOND-ORDER MOMENTS

Since we are interested in the convective flux, we must construct an equation for $\overline{u_j \theta}$. Multiplying equation (31) by θ, equation (32b) by u_i, and summing the results and averaging, we obtain (for ease of notation, we shall omit temporarily the g/c_p term in eq. [32b], and reinstate it at the end):

$$\frac{D}{Dt} \overline{u_i \theta} = -\overline{u_i u_j} \frac{\partial T}{\partial x_j} - \overline{\theta u_j} \frac{\partial U_i}{\partial x_j} + \lambda_i \overline{\theta^2} - \Pi_i^\theta - \frac{\partial}{\partial x_j} \overline{\theta u_i u_j} + \eta_i - 2\epsilon_{ijk} \Omega_j \overline{u_k \theta} , \tag{34a}$$

where

$$\Pi_i^\theta \equiv \overline{\theta \frac{\partial p}{\partial x_i}} , \qquad \eta_i \equiv \overline{\nu \theta \frac{\partial^2 u_i}{\partial x_j^2}} + \chi \overline{u_i \frac{\partial^2 \theta}{\partial x_j^2}} . \tag{34b}$$

We shall write the vector η_i as

$$\eta_i = \frac{1}{2}(\nu + \chi)\frac{\partial^2}{\partial x_j^2}\overline{u_i\theta} - \eta_i^{u\theta}, \tag{34c}$$

with

$$\eta_i^{u\theta} = (\nu + \chi)\overline{\frac{\partial\theta}{\partial x_j}\frac{\partial u_i}{\partial x_j}} - \frac{1}{2}(\nu - \chi)\left[\frac{\partial}{\partial x_j}\left(\overline{\theta\frac{\partial u_i}{\partial x_j}}\right) - \frac{\partial}{\partial x_j}\left(\overline{u_i\frac{\partial\theta}{\partial x_j}}\right)\right]. \tag{34d}$$

Following arguments first presented by Lumley, Zeman, & Siess (1978), the first term in equation (34d) is nonzero only for large Prandtl numbers which, however, are not found in stellar interiors. The second term can also be considered small on the grounds that θ and $\partial u_i/\partial x_j$ peak at different wavenumbers, and their product has little overlap. We shall therefore propose to take $\eta_i^{u\theta} \sim 0$ and so the vector η_i is given by the first term in equation (34c) only.

Next, we derive the equations for $\overline{u_i u_j}$ and $\overline{\theta^2}$. Using equations (31) and (32b), we have

$$\frac{D\overline{\theta^2}}{Dt} = -2\overline{u_i\theta}\frac{\partial T}{\partial x_i} - \frac{\partial}{\partial x_i}\overline{u_i\theta^2} + \chi\frac{\partial^2\overline{\theta^2}}{\partial x_j^2} - 2\epsilon_\theta. \tag{35a}$$

$$\frac{D}{Dt}\overline{u_i u_j} = -\left(\overline{u_j u_k}\frac{\partial U_i}{\partial x_k} + \overline{u_i u_k}\frac{\partial U_j}{\partial x_k}\right) - \frac{\partial}{\partial x_k}\left(\overline{u_i u_j u_k} + \frac{2}{3}\delta_{ij}\overline{pu_k}\right) + \lambda_i\overline{u_j\theta} + \lambda_j\overline{u_i\theta} - \Pi_{ij} + \nu\frac{\partial^2}{\partial x_k^2}\overline{u_i u_j} - \epsilon_{ij} - 2\Omega_{ij}, \tag{35b}$$

Equation (35b) was first obtained by Chou (1945). We have defined

$$\Pi_{ij} \equiv \overline{u_i\frac{\partial p}{\partial x_j}} + \overline{u_j\frac{\partial p}{\partial x_i}} - \frac{2}{3}\delta_{ij}\frac{\partial}{\partial x_k}\overline{pu_k}, \qquad \Omega_{ij} \equiv (\epsilon_{i\ell k}\overline{u_j u_k} + \epsilon_{j\ell k}\overline{u_i u_k})\Omega_\ell, \tag{35c}$$

$$\epsilon_\theta \equiv \chi\overline{\left(\frac{\partial\theta}{\partial x_j}\right)^2}, \qquad \epsilon_{ij} \equiv 2\nu\overline{\frac{\partial u_i}{\partial x_k}\frac{\partial u_j}{\partial x_k}} = \frac{2}{3}\delta_{ij}\epsilon. \tag{35d}$$

In § 8 we shall derive the dynamic equations for ϵ and ϵ_θ. Of special interest is the equation for the turbulent kinetic energy $e \equiv \frac{1}{2}\overline{q^2}$ where $q^2 \equiv u_i u_i$,

$$\frac{D}{Dt}\frac{1}{2}\overline{q^2} = -\overline{u_i u_j}\frac{\partial U_i}{\partial x_j} - \frac{\partial}{\partial x_i}\left(\frac{1}{2}\overline{q^2 u_i} + \overline{pu_i}\right) + \lambda_i\overline{u_i\theta} + \nu\frac{\partial^2 e}{\partial x_j^2} - \epsilon - \Omega_{ii}. \tag{35e}$$

5. THIRD-ORDER MOMENTS

For many years, it was customary to employ the down-gradient approximation (Donaldson 1973; Launder, Reece, & Rodi 1975)

$$\overline{u_i u_j u_k} \sim -\nu_t\frac{\partial}{\partial x_k}\overline{u_i u_j}, \tag{36a}$$

$$\overline{u_i u_j\theta} \sim -\nu_t\frac{\partial}{\partial x_j}\overline{u_i\theta}, \tag{36b}$$

$$\overline{u_i\theta^2} \sim -\nu_t\frac{\partial}{\partial x_i}\overline{\theta^2}, \tag{36c}$$

where ν_t is a turbulent or eddy viscosity usually written as the product of a typical length times a velocity. The rationale behind this type of approximation was an extension of the second-order closure whereby one takes

$$\overline{u_i u_j} \sim -\nu_t\frac{\partial U_i}{\partial x_j}. \tag{36d}$$

Equations (36a–36c) have been recently criticized for their unphysical implications, even though they are still frequently used in many geophysical studies. For example, they have been employed in the well-known treatment of the planetary boundary layer by Mellor & Yamada (1982), which has been altogether quite successful in describing the mean properties of the flow. Of 23 papers recently reviewed by Moeng & Wyngaard (1989), all but four employ the down-gradient approximation.

The original motivation was best expressed by Lumley & Khajeh-Nouri (1974): "if a crude approximation for the second-order moments [eq. (36d)] predicts first-order moments adequately, perhaps a crude approximation for third-order moments [eqs. (36a–36c)] will predict second-order moments adequately." This has however not been the case, especially in the presence of strong convective motions which are the ones of interest here. For example, planetary boundary layer data show that (Wyngaard 1973)

$$\overline{w^3} > 0, \qquad \frac{\partial}{\partial z}\overline{w^2} > 0, \tag{36e}$$

whereas the down-gradient approximation (eq. [36]) implies just the opposite. Zeman & Lumley (1976) have pointed out other shortcomings for the kinetic energy flux. The main physical ingredient not accounted for by the down-gradient approximation is *buoyancy*. Moeng & Wyngaard (1989) using large eddy simulation (LES) data have shown that buoyancy effects give the largest contribution to $\overline{w^2\theta}$ and/or $\overline{w^2 q}$, whereas the down-gradient approximation accounts for the smallest of all contributions. The conclusion is that, in the case of strong convection, one must bypass the down-gradient approximation and consider the full expression for the third-order moments (Finger & Schmidt 1986).

Using the basic equations derived above, we derive the following results:

$$\frac{D}{Dt}\overline{u_i u_j u_k} = -\left(\overline{u_i u_j u_\ell}\frac{\partial U_k}{\partial x_\ell} + \text{perm.}\right) + \left(\overline{u_i u_j}\frac{\partial}{\partial x_\ell}\overline{u_k u_\ell} + \text{perm.}\right) - \frac{\partial}{\partial x_\ell}\overline{u_i u_j u_k u_\ell} + (\lambda_i \overline{u_j u_k \theta} + \text{perm.}) - \Pi_{ijk} - 2\Omega_{ijk} - \epsilon_{ijk} + \nu\frac{\partial^2}{\partial x_\ell^2}(\overline{u_i u_j u_k}) , \tag{37a}$$

where

$$\Pi_{ijk} = \overline{u_i u_j \frac{\partial p}{\partial x_k}} + \text{perm.} , \tag{37b}$$

$$\Omega_{ijk} = (\epsilon_{i\ell m}\overline{u_j u_k u_m} + \text{perm.})\Omega_\ell , \tag{37c}$$

$$\epsilon_{ijk} \equiv 2\nu\left(\overline{u_i \frac{\partial u_j}{\partial x_\ell}\frac{\partial u_k}{\partial x_\ell}} + \text{perm.}\right) . \tag{37d}$$

Using the definition of the tensor ϵ_{ij} (eq. [35d]), we shall write the tensor ϵ_{ijk} as

$$\epsilon_{ijk} \approx \overline{u_i \epsilon_{jk}} + \text{perm.} = \frac{2}{3}(\delta_{jk}\overline{u_i \epsilon} + \text{perm.}) = \frac{2}{3\tau}(\delta_{jk}\overline{q^2 u_i} + \text{perm.}) , \tag{37e}$$

where we have used the relations

$$\overline{u_i \epsilon} = \tau^{-1}\overline{q^2 u_i} , \qquad \tau \equiv \overline{q^2}/\epsilon . \tag{37f}$$

Analogously, one derives

$$\frac{D}{Dt}\overline{u_i u_j \theta} = -\overline{u_i u_j u_\ell}\frac{\partial T}{\partial x_\ell} - \left(\overline{u_i u_\ell \theta}\frac{\partial U_j}{\partial x_\ell} + \overline{u_j u_\ell \theta}\frac{\partial U_i}{\partial x_\ell}\right) - \frac{\partial}{\partial x_\ell}\overline{u_i u_j u_\ell \theta} + \overline{u_i u_j}\frac{\partial}{\partial x_\ell}\overline{\theta u_\ell} + \overline{\theta u_i}\frac{\partial}{\partial x_\ell}\overline{u_j u_\ell} + \overline{\theta u_j}\frac{\partial}{\partial x_\ell}\overline{u_i u_\ell} + \lambda_i \overline{\theta^2 u_j} + \lambda_j \overline{\theta^2 u_i} - \Pi_{ij}^\theta - 2\Lambda_{ij} + \eta_{ij} , \tag{38a}$$

where

$$\Pi_{ij}^\theta \equiv \overline{\theta u_i \frac{\partial p}{\partial x_j}} + \overline{\theta u_j \frac{\partial p}{\partial x_i}} , \tag{38b}$$

$$\Lambda_{ij} \equiv (\epsilon_{i\ell k}\overline{u_j u_k \theta} + \epsilon_{j\ell k}\overline{u_i u_k \theta})\Omega_\ell , \tag{38c}$$

$$\eta_{ij} = \nu\left(\overline{\theta u_i \frac{\partial^2 u_j}{\partial x_\ell^2}} + \overline{\theta u_j \frac{\partial^2 u_i}{\partial x_\ell^2}}\right) + \chi\overline{u_i u_j \frac{\partial^2 \theta}{\partial x_\ell^2}} . \tag{38d}$$

The tensor η_{ij} is considerably more difficult to handle than any of the previous dissipation terms, and we can therefore only offer formulae that are not fully rigorous, but rather based on physical arguments. Consider the first parentheses in equation (38d): we shall rewrite it as

$$\overline{\theta \frac{\partial^2}{\partial x_\ell^2} u_i u_j} - 2\overline{\theta \frac{\partial u_i}{\partial x_\ell}\frac{\partial u_j}{\partial x_\ell}} .$$

While the first term may be considered small because the two terms peak at different wavenumbers, the last term may be written, using the tensor ϵ_{ij}, as

$$-\nu^{-1}\overline{\theta\epsilon_{ij}} = -\nu^{-1}\tfrac{2}{3}\delta_{ij}\tau^{-1}\overline{q^2\theta} . \tag{38e}$$

Introducing the time scale τ_θ defined as

$$\tau_\theta = \overline{\theta^2}/\epsilon_\theta , \tag{38f}$$

one can perform a similar analysis of the second term in equation (38d). Collecting the results, we finally obtain

$$\eta_{ij} \approx -\frac{2}{3\tau}\left(1+\frac{3}{2}\frac{\tau}{\tau_\theta}\right)\delta_{ij}\overline{q^2\theta}\,,$$

which we shall rewrite as

$$\eta_{ij} = -\frac{2}{3\tau}\,c_{10}\,\delta_{ij}\overline{q^2\theta}\,. \tag{38g}$$

André et al. (1978) and André, Lacarrere, & Traoré (1982) have suggested a similar result with the value $c_{10} = 6$.

Next we consider the quantity $\overline{u_i\theta^2}$ for which the dynamic equation is derived to be

$$\frac{D}{Dt}\overline{u_i\theta^2} = -2\overline{\theta u_i u_j}\frac{\partial T}{\partial x_j} - \overline{u_j\theta^2}\frac{\partial U_i}{\partial x_j} + \overline{\theta^2}\frac{\partial}{\partial x_j}\overline{u_i u_j} + 2\overline{\theta u_i}\frac{\partial}{\partial x_j}\overline{\theta u_j} - \frac{\partial}{\partial x_j}\overline{\theta^2 u_i u_j} - \Pi_i^{\theta\theta} + \lambda_i\overline{\theta^3} - 2\epsilon_{ijk}\Omega_j\overline{u_k\theta^2} + \omega_i\,, \tag{39a}$$

where

$$\Pi_i^{\theta\theta} = \overline{\theta^2\frac{\partial p}{\partial x_i}}\,, \qquad \omega_i \equiv \nu\overline{\theta^2\frac{\partial^2 u_i}{\partial x_j^2}} + 2\chi\overline{\theta u_i\frac{\partial^2\theta}{\partial x_j^2}}\,. \tag{39b}$$

As before, the vector ω_i will be treated only approximately in the hope of getting the major physical contribution. First, we propose to neglect the first term because of the vanishing viscosity and the fact that θ^2 and $\partial^2 u_i/\partial x_k^2$ peak at different wavenumber; as for the second term, we shall write it as

$$2\chi\left[\overline{u_i\frac{\partial}{\partial x_j}\left(\theta\frac{\partial\theta}{\partial x_j}\right)} - \overline{u_i\left(\frac{\partial\theta}{\partial x_j}\right)^2}\right] \approx -2\overline{\epsilon_\theta u_i}\,, \tag{39c}$$

so that finally

$$\omega_i = -2\overline{\epsilon_\theta u_i} = -2\tau_\theta^{-1}\overline{\theta^2 u_i}\,, \tag{39d}$$

where, in analogy with equation (37f), one takes

$$\overline{\epsilon_\theta u_i} = \tau_\theta^{-1}\overline{\theta^2 u_i}\,. \tag{39e}$$

For completeness, we also derive the equation for $\overline{\theta^3}$,

$$\frac{D}{Dt}\overline{\theta^3} = -3\overline{\theta^2 u_j}\frac{\partial T}{\partial x_j} - \frac{\partial}{\partial x_j}\overline{\theta^3 u_j} + 3\overline{\theta^2}\frac{\partial}{\partial x_j}\overline{\theta u_j} + \chi\frac{\partial^2}{\partial x_k^2}\overline{\theta^3} - \epsilon_{\theta\theta\theta}\,, \tag{40a}$$

where

$$\epsilon_{\theta\theta\theta} \equiv 6\chi\overline{\theta\left(\frac{\partial\theta}{\partial x_j}\right)^2} = \left(\frac{2c_{10}}{\tau}\right)\overline{\theta^3}\,, \tag{40b}$$

and where the last step is based on a suggestion by André et al. (1978, 1982).

6. FOURTH-ORDER MOMENTS

As expected, the third-order correlations imply the fourth-order correlations

$$\overline{u_i u_j u_k u_\ell}\,, \qquad \overline{u_i u_j u_k\theta}\,, \qquad \overline{\theta^2 u_i u_j}\,.$$

Like previous authors, we shall adopt the Hanjalic & Launder (1972, 1976) approximation discussed in detail by Zeman (1981). This consists of taking the fourth-order moments to be jointly Gaussian distributed but replacing the pressure correlations, which are integrals of fourth-order products, by third-order terms divided by a time scale that, following other authors, we shall denote by τ_3. Lumley et al. (1978) have pointed out that the Hanjalic-Launder approximation is physically equivalent to the EDQNM model (Orszag 1977; Lesieur 1990). We shall therefore assume that for any $\overline{abcd}$ we have

$$\overline{abcd} = \overline{ab}\,\overline{cd} + \overline{ac}\,\overline{bd} + \overline{ad}\,\overline{bc}\,, \tag{41}$$

which will allow us to express the third-order correlations in terms of the second-order correlations.

7. PRESSURE CORRELATION TERMS

Both the second- and third-order moments contain the pressure correlation terms Π_i^θ and Π_{ij} (eqs. [34b] and [35c]), which must be specified before the equations can be solved. Both terms have been the subject of much work over the years (Lumley 1978; Lumley et al. 1978; Lumley & Khajeh-Nouri 1974). To begin, let us take the divergence of the momentum equations for u_i (eq. [31]). The result is the following Poisson equation (no rotation):

$$\frac{\partial^2 p}{\partial x_i^2} = \frac{\partial^2}{\partial x_i\partial x_j}(\overline{u_i u_j} - u_i u_j) - 2\frac{\partial U_i}{\partial x_j}\frac{\partial u_j}{\partial x_i} - \lambda_i\frac{\partial\theta}{\partial x_i}\,. \tag{42}$$

Pressure fluctuations thus arise from three sources: turbulence-turbulence interaction (first term), turbulence-mean flow interaction (second term), and buoyancy forces (last term). In the absence of the last term, Launder et al. (1975) suggested that the tensor Π_{ij} be constructed so as to mirror the contributions in the Poisson equation. Thus, for the deviatoric (traceless) part, they proposed the form

$$\Pi_{ij} = 2c_1\tau^{-1}(\overline{u_i u_j} - \tfrac{1}{3}\overline{q^2}\delta_{ij}) + c_2(P_{ij} - \tfrac{1}{3}P\,\delta_{ij}) ,$$

with

$$P_{ij} = -\left(\overline{u_i u_k}\,\frac{\partial U_j}{\partial x_k} + \overline{u_j u_k}\,\frac{\partial U_i}{\partial x_k}\right) ,$$

and P is the trace of P_{ij}. Historically, the first term in Π_{ij} was proposed by Rotta (1951) and is called "return-to-isotropy," for Rotta suggested that "collisions" among (large) eddies would promote a return to isotropy proportional to the prevailing level of anisotropy. The second term in Π_{ij} was first proposed by Naot, Shavit, & Wolfshtein (1973) and later discussed by Launder (1975), who pointed out that once the importance of the second term is accepted, "it is difficult not to conclude that an analogous term arising from buoyancy forces not be included." He then proposed a "rational extension" of the form

$$P_{ij} \to P_{ij} - (\lambda_i\overline{\theta u_j} + \lambda_j\overline{\theta u_i}) .$$

Analogous reasoning applied to the vector Π_i^θ (eq. [34b]) suggested a structure of the form (Launder 1975)

$$\Pi_i^\theta = 2c_1\tau^{-1}\overline{u_i\theta} - c_2\left(\overline{u_k\theta}\,\frac{\partial U_i}{\partial x_k} + \lambda_i\overline{\theta^2}\right) .$$

At the same time, Zeman & Tennekes (1975) pointed out the need to include in Π_{ij} vorticity terms and thus the need to include a new tensor in the expression for Π_{ij}. In what follows, we shall give the general expressions for Π_i and Π_{ij} and then compare them with the forms suggested by different authors. In the ordering of terms, we follow Zeman & Lumley (1979):

$$\Pi_i^\theta = \Pi_{i1}^\theta + \Pi_{i2}^\theta , \tag{43}$$

$$\Pi_{i1}^\theta = 2c_6\tau^{-1}\overline{u_i\theta} + c_7\alpha g\overline{\theta^2}\,\delta_{3i} , \tag{43a}$$

$$\Pi_{i2}^\theta = -\frac{4}{5}\,a_m\left(\frac{\partial U_k}{\partial x_j} - 2\epsilon_{kjm}\Omega_m\right)\left[\delta_{ik}\overline{\theta u_j} - \frac{1}{4}\,(\delta_{kj}\overline{\theta u_i} + \delta_{ij}\overline{\theta u_k})\right] , \tag{43b}$$

and for the traceless tensor Π_{ij},

$$\Pi_{ij} = \Pi_{ij}^{(1)} + \Pi_{ij}^{(2)} , \tag{44}$$

$$\Pi_{ij}^{(1)} = 2c_4\tau^{-1}b_{ij} + c_5\,g\alpha(\delta_{3i}\overline{\theta u_j} + \delta_{3j}\overline{\theta u_i} - \tfrac{2}{3}\delta_{ij}\overline{\theta w}) , \tag{44a}$$

$$-\Pi_{ij}^{(2)} = \tfrac{4}{3}\alpha_0\,eS_{ij} + 2\alpha_1(S_{ik}b_{kj} + S_{kj}b_{ik} - \tfrac{2}{3}\delta_{ij}S_{k\ell}b_{\ell k}) + 2\alpha_2(R_{ik}b_{kj} + R_{jk}b_{ik} - \tfrac{2}{3}\delta_{ij}R_{k\ell}b_{\ell k}) \tag{44b}$$

where

$$b_{ij} \equiv \overline{u_i u_j} - \tfrac{1}{3}\overline{q^2}\,\delta_{ij} ,$$

$$2S_{ij} \equiv \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} , \qquad 2R_{ij} \equiv \frac{\partial U_i}{\partial x_j} - \frac{\partial U_j}{\partial x_i} - 4\epsilon_{ijk}\Omega_k . \tag{44c}$$

Zeman & Lumley (1979) suggested (see, however, Gerz, Schumann, & Elghobashi 1989)

$$2c_4 = 3.5 , \quad c_5 = \tfrac{3}{10} , \quad 2c_6 = 7.5 , \quad c_7 = \tfrac{1}{3}, \tfrac{1}{5} , \quad \alpha_0 = \tfrac{3}{5} , \quad \alpha_1 = 0.31 , \quad \alpha_2 = 0.22 , \quad a_m = 0.56 . \tag{44d}$$

The other pressure correlation terms are taken to be (André et al. 1982)

$$\Pi_{ijk} = 2c_8\tau^{-1}\overline{u_i u_j u_k} + c_{11}(\overline{u_i u_j\theta}\,\lambda_k + \text{perm.}) , \tag{44e}$$

$$\Pi_{ij}^\theta = 2c_8\,\tau^{-1}\overline{u_i u_j\theta} + c_{11}(\lambda_j\overline{u_i\theta^2} + \lambda_i\overline{u_j\theta^2} - \tfrac{2}{3}\delta_{ij}\lambda_k\overline{u_k\theta^2}) - \tfrac{2}{3}\tau^{-1}(c_8 + 3c_9)\overline{q^2\theta}\,\delta_{ij} , \tag{44f}$$

$$\Pi_i^{\theta\theta} = 2c_8\tau^{-1}\overline{u_i\theta^2} + c_{11}\lambda_i\overline{\theta^3} . \tag{45}$$

8. DISSIPATION TERMS

The equation for ϵ is usually written as (Lumley & Khajeh-Nouri 1974; Zeman 1975; Zeman & Lumley 1976; Lumley 1978; Launder 1990)

$$\frac{D}{Dt}\,\epsilon + \frac{\partial}{\partial x_j}\,(\overline{\epsilon u_j}) = a_1\tau^{-1}(P_\theta + P_s) - a_2\,\epsilon\tau^{-1} , \tag{46}$$

with $a_1 = 1.44$, $a_2 = 3.8$, and

$$P_\theta = \text{trace of: } P_{ij}^\theta = \lambda_i\overline{\theta u_j} + \lambda_j\overline{\theta u_i} , \tag{47}$$

$$P_s = \text{trace of: } P_{ij} = -\left(\overline{u_i u_k}\,\frac{\partial U_j}{\partial x_k} + \overline{u_j u_k}\,\frac{\partial U_i}{\partial x_k}\right). \tag{48}$$

The standard form of equation (46) without buoyancy (e.g., Speziale 1991) may look slightly different from equation (46); however, assuming τ to be constant, one has $\partial q^2/\partial z = (q^2/\epsilon)\partial\epsilon/\partial z$, and so, using equation (37f),

$$\overline{\epsilon w} = \tau^{-1}\left[\overline{q^2 w}\Big/\left(\frac{\partial}{\partial z}\,\overline{q^2}\right)\right]\frac{\partial}{\partial z}\,\overline{q^2} = -\kappa_t\,\frac{\partial \epsilon}{\partial z}\,, \tag{49}$$

$$\kappa_t = -\overline{q^2 w}(\partial\overline{q^2}/\partial z)^{-1}\,, \tag{50}$$

which makes equation (46) look like its standard form. Since κ_t has dimensions of $w\ell$, a dimensional argument applied to equation (46) yields

$$\epsilon \sim \frac{e^{3/2}}{\ell}\,. \tag{51}$$

The major disadvantage of equation (51) is that it does not prescribe the mixing length ℓ, the choice of which, however, is crucial. The equation for ϵ_θ is given by (Zeman & Lumley 1979)

$$\frac{D}{Dt}\,\epsilon_\theta + \frac{\partial}{\partial x_j}\,(\overline{\epsilon_\theta u_j}) = -b_1\epsilon_\theta\tau_\theta^{-1}\left(1 + \frac{1}{4}\,\frac{\tau_\theta}{\tau}\right) + b_2(\epsilon\tau^3)^{-1}(\overline{w\theta})^2 - b_3\tau_\theta^{-1}\,\overline{w\theta}\,\frac{\partial T}{\partial z} + \chi\nabla^2\epsilon_\theta\,, \tag{52}$$

where the relations analogous to equations (49) and (50) are

$$\overline{\epsilon_\theta w} = -K_h\,\frac{\partial}{\partial z}\,\epsilon_\theta\,, \qquad K_h = -\overline{\theta^2 w}\left(\frac{\partial\overline{\theta^2}}{\partial z}\right)^{-1}\,. \tag{53}$$

The suggested values of the constants are $b_1 = 3$, $b_2 = 30$, and $b_3 = 0.97$. It must be noted that some authors (e.g., André et al. 1982) have used the much simpler relation ($c_2 = 5/2$)

$$\epsilon_\theta = 2c_2\tau^{-1}\overline{\theta^2}\,. \tag{54}$$

9. EQUATIONS FOR THE THIRD-ORDER MOMENTS

Using equations (41), (44e–44f), and (45), equations (37a), (38a), (39a), and (40a) become

$$\left(\frac{D}{Dt} + \tau_3^{-1}\right)\overline{u_i u_j u_k} = -\left(\overline{u_i u_j u_\ell}\,\frac{\partial U_k}{\partial x_\ell} + \text{perm.}\right) - \left(\overline{u_i u_\ell}\,\frac{\partial}{\partial x_\ell}\,\overline{u_j u_k} + \text{perm.}\right) + (1 - c_{11})(\lambda_i\overline{\theta u_j u_k} + \text{perm.})$$
$$- 2\Omega_{ijk} - \frac{2}{3\tau}\,(\delta_{ij}\overline{q^2 u_k} + \text{perm.}) + \nu\,\frac{\partial^2}{\partial x_\ell^2}\,(\overline{u_i u_j u_k})\,, \tag{55a}$$

$$\left(\frac{D}{Dt} + \tau_3^{-1}\right)\overline{u_i u_j \theta} = -\overline{u_i u_j u_k}\,\frac{\partial T}{\partial x_k} - \left(\overline{u_i u_k \theta}\,\frac{\partial U_j}{\partial x_k} + \overline{u_j u_k \theta}\,\frac{\partial U_i}{\partial x_k}\right) - \left(\overline{u_i u_k}\,\frac{\partial}{\partial x_k}\,\overline{\theta u_j} + \overline{u_j u_k}\,\frac{\partial}{\partial x_k}\,\overline{\theta u_i} + \overline{\theta u_k}\,\frac{\partial}{\partial x_k}\,\overline{u_i u_j}\right)$$
$$+ \frac{2}{3}\,c_{11}\delta_{ij}\lambda_k\overline{\theta^2 u_k} + \tau^{-1}c_*\delta_{ij}\overline{q^2\theta} + (1 - c_{11})(\lambda_i\overline{\theta^2 u_j} + \lambda_j\overline{\theta^2 u_i}) - 2\Lambda_{ij}\,, \tag{55b}$$

$$\left(\frac{D}{Dt} + \tau_3^{-1} + 2\tau_\theta^{-1}\right)\overline{u_i\theta^2} = -2\overline{\theta u_i u_j}\,\frac{\partial T}{\partial x_j} - \overline{\theta^2 u_j}\,\frac{\partial U_i}{\partial x_j} - 2\overline{\theta u_j}\,\frac{\partial}{\partial x_j}\,\overline{\theta u_i} + (1 - c_{11})\lambda_i\overline{\theta^3} - \overline{u_i u_j}\,\frac{\partial}{\partial x_j}\,\overline{\theta^2} - 2\epsilon_{ijk}\Omega_j\overline{u_k\theta^2}\,, \tag{55c}$$

$$\left(\frac{D}{Dt} + \frac{c_{10}}{c_8}\,\tau_3^{-1}\right)\overline{\theta^3} = -3\overline{\theta^2 u_j}\,\frac{\partial T}{\partial x_j} - 3\overline{\theta u_j}\,\frac{\partial}{\partial x_j}\,\overline{\theta^2} + \chi\,\frac{\partial^2}{\partial x_\ell^2}\,\overline{\theta^3}\,, \tag{55d}$$

where $c_* = (2/3)(c_8 + 3c_9 - c_{10})$. Lumley et al. (1978) have taken $c_{11} = 3/10$ and $c_* = 1$, whereas, due to realizability requirements, André et al. (1982) concluded that $c_* = 0$. In writing equations (55), we have used the notation (Zeman 1975, 1981)

$$\tau_3 \equiv \tau/2c_8\,, \tag{55e}$$

André et al. (1982) have suggested $c_8 = 8$, $c_9 = -0.67$, $c_{10} = 6$, and $c_{11} = \frac{1}{5}$.

10. TURBULENT CONVECTION

In the case of pure convection, we shall take $\boldsymbol{U} = 0$ and also neglect rotation and viscosity. Using equations (43), (44), and (Lumley 1978)

$$\overline{pw} = -a\overline{wq^2}\,, \tag{56}$$

with $a = \frac{1}{5}$, the equations for the second-order moments, that is, equations (34a), (35a), (35b), (35f), and (55), become, after reinstating the g/c_p term and using equation (3), the following:

Convective flux:

$$\frac{\partial}{\partial t}\overline{w\theta}+\frac{\partial}{\partial z}\overline{\theta w^2}=\beta\overline{w^2}+(1-c_7)g\alpha\overline{\theta^2}-2c_6\tau^{-1}\overline{w\theta}+\frac{1}{2}\chi\frac{\partial^2}{\partial z^2}\overline{w\theta}\,; \tag{57}$$

Turbulent temperature:

$$\frac{\partial}{\partial t}\overline{\theta^2}+\frac{\partial}{\partial z}\overline{w\theta^2}=2\beta\overline{w\theta}+\chi\frac{\partial^2\overline{\theta^2}}{\partial z^2}-2\epsilon_\theta\,; \tag{58}$$

Momentum flux:

$$\frac{\partial}{\partial t}\overline{w^2}+\frac{\partial}{\partial z}\left(\overline{w^3}-\frac{2}{3}a\overline{q^2w}\right)=-2c_4\tau^{-1}\left(\overline{w^2}-\frac{1}{3}\overline{q^2}\right)+2\left(1-\frac{2}{3}c_5\right)g\alpha\overline{\theta w}-\frac{2}{3}\epsilon\,; \tag{59}$$

Turbulent kinetic energy:

$$\frac{\partial}{\partial t}\frac{1}{2}\overline{q^2}+\left(\frac{1}{2}-a\right)\frac{\partial}{\partial z}\overline{q^2w}=g\alpha\overline{w\theta}-\epsilon\,. \tag{60}$$

To solve these equations, one needs the third-order moments $\overline{w^2\theta}$, $\overline{w\theta^2}$, $\overline{w^3}$, $\overline{q^2w}$, which in turn entail two more moments, $\overline{\theta^3}$ and $\overline{q^2\theta}$, whose equations are given by equations (55), that is,

$$\left(\frac{\partial}{\partial t}+\tau_3^{-1}\right)\overline{w^2\theta}=\beta\overline{w^3}-\overline{w\theta}\frac{\partial}{\partial z}\overline{w^2}+2\left(1-\frac{2}{3}c_{11}\right)g\alpha\overline{w\theta^2}-2\overline{w^2}\frac{\partial}{\partial z}\overline{w\theta}+\tau^{-1}c_*\overline{q^2\theta}\,, \tag{61}$$

$$\left(\frac{\partial}{\partial t}+\tau_3^{-1}+2\tau_\theta^{-1}\right)\overline{w\theta^2}=2\beta\overline{\theta w^2}-2\overline{\theta w}\frac{\partial}{\partial z}\overline{\theta w}-\overline{w^2}\frac{\partial}{\partial z}\overline{\theta^2}+(1-c_{11})g\alpha\overline{\theta^3}\,, \tag{62}$$

$$\left(\frac{\partial}{\partial t}+\tau_3^{-1}\right)\overline{w^3}=-3\overline{w^2}\frac{\partial}{\partial z}\overline{w^2}+3(1-c_{11})g\alpha\overline{\theta w^2}-2\tau^{-1}\overline{q^2w}\,, \tag{63}$$

$$\left(\frac{\partial}{\partial t}+\tau_3^{-1}+\frac{10}{3}\tau^{-1}\right)\overline{q^2w}=-\left(2\overline{w^2}\frac{\partial}{\partial z}\overline{w^2}+\overline{w^2}\frac{\partial}{\partial z}\overline{q^2}\right)+(1-c_{11})g\alpha(2\overline{\theta w^2}+\overline{q^2\theta})\,, \tag{64}$$

$$\left(\frac{\partial}{\partial t}+\tau_3^{-1}\right)\overline{q^2\theta}=\beta\overline{q^2w}+2g\alpha\overline{\theta^2w}-\left(2\overline{w^2}\frac{\partial}{\partial z}\overline{w\theta}+\overline{w\theta}\frac{\partial}{\partial z}\overline{q^2}\right)+3c_*\tau^{-1}\overline{q^2\theta}\,, \tag{65}$$

$$\left(\frac{\partial}{\partial t}+\frac{c_{10}}{c_8}\tau_3^{-1}\right)\overline{\theta^3}=3\beta\overline{w\theta^2}-3\overline{w\theta}\frac{\partial}{\partial z}\overline{\theta^2}+\chi\frac{\partial^2}{\partial z^2}\overline{\theta^3}\,. \tag{66}$$

We have neglected terms like $\overline{uw}(\overline{uw})'$, $\overline{uw}(\overline{u\theta})'$ compared to $\overline{w^2}(\overline{w^2})'$ and $\overline{w^2}(\overline{w\theta})'$, respectively. The equations for ϵ and ϵ_θ are equations (46) and (52).

11. THE TEMPERATURE PROFILE

The complete model, equations (57)–(66) plus equations (46) and (52) for ϵ and ϵ_θ, contains the function β, the gradient of the true temperature profile, defined by (see eq. [3])

$$\beta=-\left(\frac{\partial T}{\partial z}+\frac{g}{c_p}\right)=-\left(\frac{\partial\Theta}{\partial z}+\frac{\partial T_0}{\partial z}+\frac{g}{c_p}\right)=\beta^0-\frac{\partial\Theta}{\partial z}\,, \tag{67}$$

with Θ given by equation (32a), that is,

$$\frac{\partial\Theta}{\partial t}+\frac{\partial}{\partial z}\overline{w\theta}=\chi\frac{\partial^2\Theta}{\partial z^2}\,. \tag{68}$$

At this point, we can proceed in either of two ways: we can neglect the time dependence in equation (68), integrate once, and then substitute $\partial\Theta/\partial z$ in equation (67). The result is

$$\beta=\beta_0-\chi^{-1}\overline{w\theta}\,, \tag{69}$$

which expresses the variable β in terms of β_0, the known temperature gradient (computed as if all the flux were transported by radiation: in Cox & Giuli 1968, eq. [14.12], it is called the fictitious radiative gradient, and in dimensionless units it is denoted by ∇_r) and of the second-order moment $\overline{w\theta}$. Therefore, once an external $\beta_0(z)$ versus z function is chosen, the set of equations (57)–(66) can be fully solved. Clearly, equation (69) is just the flux conservation, equation (33).

Another, more exact, way of proceeding is by way of keeping the time dependence in equation (68). Eliminating Θ using equation (67), one obtains the time evolution equation for the function β:

$$\frac{\partial \beta}{\partial t} = \chi \frac{\partial^2 \beta}{\partial z^2} + \frac{\partial^2}{\partial z^2} \overline{w\theta} - \chi \frac{\partial^2 \beta^0}{\partial z^2} . \tag{70}$$

We may note that from equation (27) we derive

$$\frac{\partial \beta^0}{\partial z} = K^{-1} Q(z) - \frac{\partial}{\partial z}\left(\frac{g}{c_p}\right) . \tag{71}$$

12. THE MLT FORMULA FOR F_c

It is instructive to derive the MLT expression (13) from the full set of equations so as to understand its range of validity. Consider equations (57)–(59) with $\chi = 0$ (maximum convective efficiency) and

$$\frac{\partial}{\partial t} = 0 , \quad \frac{\partial}{\partial z}(\overline{w^3}, \overline{wq^2}) = 0 , \quad \frac{\partial}{\partial z}(\overline{\theta w^2}, \overline{w\theta^2}) = 0 , \quad \overline{\theta^2} = 0 , \tag{72}$$

that is, in the absence of third-order moments and temperature variance. At the same time, equation (46) will be used in its simplified form (51), which we shall write as

$$\epsilon = c_\epsilon e^{3/2} \ell^{-1} , \tag{73a}$$

where the constant c_ϵ is taken from Schmidt & Schumann (1989, hereafter SS89) to be

$$c_\epsilon = \pi\left(\frac{2}{3\,\mathrm{Ko}}\right)^{3/2} = 0.845 , \tag{73b}$$

with the Kolmogorov constant Ko taken to be 1.6; as before, ℓ and e are the mixing length and the turbulent kinetic energy. It then follows that

$$\tau = 2e\epsilon^{-1} = \frac{2}{c_\epsilon} \frac{\ell}{e^{1/2}} . \tag{74}$$

Substituting $\overline{w^2}$ from equation (59) into equation (57), we obtain

$$\overline{w\theta} = \kappa_t \beta , \tag{75a}$$

where the turbulent conductivity κ_t is given by

$$\kappa_t = A_1 e^{1/2} \ell (1 - A_2 \ell^2 N^2 e^{-1})^{-1} , \tag{75b}$$

and where the constants A are defined as

$$3c_6 c_\epsilon A_1 \equiv 2(1 - c_4^{-1}) , \qquad c_6 c_4 c_\epsilon^2 A_2 \equiv 2(1 - \tfrac{2}{3} c_5) , \tag{75c}$$

and where N is Brunt-Vaisala frequency

$$N^2 = g\alpha\beta = \left(\frac{g}{H_p}\right)(\nabla - \nabla_{\mathrm{ad}}) . \tag{76}$$

Finally, use of equation (60) gives

$$\epsilon = g\alpha\overline{w\theta} . \tag{77}$$

Equations (75), (77), and (73a) yield for the kinetic energy e,

$$e = A_3 \ell^2 N^2 , \tag{78}$$

with $A_3 \equiv A_2 + A_1/c_\epsilon$. Substitution of equation (78) into equation (75a) yields the convective flux (1)

$$\overline{w\theta} = C(g\alpha)^{1/2} \ell^2 \beta^{3/2} , \tag{79}$$

with $C \equiv c_\epsilon A_3^{3/2}$. Equation (79) coincides with equation (13).

13. COUNTERGRADIENT

Here, we shall relax the last two conditions (72) and investigate their effect. Repeating a calculation similar to the one in § 12, one obtains

$$\overline{w\theta} = \kappa_t\left(-\frac{\partial T'}{\partial z} + \Gamma_c\right) , \tag{80}$$

$$\Gamma_c \sim g\alpha \frac{\overline{\theta^2}}{e} > 0 , \tag{81}$$

where we have used the simplified notation

$$\frac{\partial T'}{\partial z} \equiv \frac{\partial T}{\partial z} - \left(\frac{\partial T}{\partial z}\right)_{\rm ad} . \tag{82}$$

In equation (80), Γ_c plays the role of a *countergradient*: *even in regions where*

$$\nabla - \nabla_{\rm ad} \leq 0 ,$$

there is a convective flux carried by Γ_c: *heat can be transported from cold to hot regions.* Deardorff (1972) proposed Γ_c as the explanation of the Priestly-Swinback effect (1947) in atmospheric turbulence. Recent relevant work has been carried out by Grotzbach (1986), Finger & Schmidt (1986), Schumann (1987), who provides an excellent physical interpretation of the phenomenon, and Holstag & Moeng (1991). The general conclusion is that the diffusion terms (divergence of third-order moments $\overline{w^2\theta}$ and $\overline{w\theta^2}$) are responsible for the countergradient.

14. OVERSHOOTING

Although the only proper way to quantify the phenomenon of overshooting is by way of solving the full set of equations presented earlier, we shall make here some general remarks. Within the context of atmospheric turbulence, this problem has been considered by several authors (Ball 1960; Tennekes 1973; Zilitinkevich 1975). The basic argument is that near the inversion zone, where the temperature gradient changes sign as one enters the stably stratified region, the dissipation ϵ in equation (60) may be neglected. Thus, the negative convective flux can be estimated from equation (60) to be

$$g\alpha(\overline{w\theta})_i \approx \left(\frac{1}{2} - a\right) \frac{\partial}{\partial z} \overline{q^2 w} \approx -\left(\frac{1}{2} - a\right) \frac{\overline{w^3}}{h} , \tag{83}$$

where h is the height of the convective layer. In a state of fully developed turbulence, the turbulent kinetic energy is maintained by buoyancy, and so one can take advantage of the exact relation (Cox & Giuli 1968, equations. [14.113–114])

$$\overline{w^3}/(g\alpha\ell\overline{w\theta}) = \text{constant} , \tag{84}$$

so that

$$(\overline{w\theta})_i \approx \text{constant} \left(\frac{1}{2} - a\right)\left(\frac{\ell}{h}\right)\overline{w\theta} , \tag{85}$$

to be compared with Tennekes expression

$$(\overline{w\theta})_i \approx -\tfrac{2}{10}(\overline{w\theta})_{\rm max} . \tag{86}$$

15. TURBULENT VISCOSITY AND CONDUCTIVITY: NUMERICAL SIMULATIONS

The advent of fast computers has made available two new research tools to investigate turbulence: DNS (direct numerical simulation) and LES (large eddy simulation). The former refers to those situations in which either the Reynolds and/or the Rayleigh numbers are sufficiently small to allow a description of all the dynamical scales (eddies). Since the number of degrees of freedom N to be accounted for can be shown to grow as Re^3 (Marcus 1986), DNS techniques cannot be applied to geophysical and/or astrophysical flows that are characterized by very large values of Re. This leaves as the only option the LES, through which one resolves the largest scales or eddies, leaving open the problem of including the effect of the smaller eddies: one needs a model for the subgrid scales (SGS). For a recent survey of LES results, see Nieuwstadt et al. (1991) and Nieuwstadt (1991). In the context of turbulent convection of astrophysical interest, Chan & Sofia (1989) and Hossain & Mullan (1991) have carried out extensive LES computations. To represent the SGS, they adopted a model whereby the smaller scales are viewed as draining energy from the largest scales via a turbulent viscosity ν_t for which the Smagorinsky model (1963) suggests

$$\nu_t = C_s^2 \Delta^2 S , \tag{87}$$

where $C_s = 0.165$, S is the shear exerted by the largest scales over the subgrid scales, and Δ is the size of the smallest scale still resolved by the LES. The spirit of equation (87) is that the contribution of the SGS is entirely written in terms of quantities like Δ and S that refer to the large scales and are therefore known. The empirical constant C_s has recently been derived from the renormalization group techniques (RNG; Yakhot & Orszag 1986).

It is generally felt that in the presence of strong buoyancy, equation (87) is incomplete since in addition to the time scale represented by the shear there should also be the buoyancy-related frequency, N (eq. [76]). In general, one would expect a formula of the type

$$\nu_t = C^2 \Delta^2 S f(\mathrm{Ri}) , \tag{88}$$

where Ri is the Richardson number $\mathrm{Ri} = N^2/S^2$; for $\mathrm{Ri} \to 0, f \to 1$, and $C \to C_s$. Using the formalism developed earlier, we shall calculate a possible form for f. To that effect, we make use of equation (75) where we further write κ_t as

$$\kappa_t = \ell_t e^{1/2} , \qquad \ell_t = A_1 \Delta (1 - A_2 \Delta^2 N^2 e^{-1})^{-1} . \tag{89}$$

Since we have included the presence of $\overline{\theta^2}$, the coefficient A_2 given by equation (75c) should be supplemented by $2(1 - c_7)(c_6 c_\epsilon c_\theta)^{-1}$, where the constant c_θ, which can be related to the Batchelor constant, has the value of 2.02 (SS89). We have also identified the length ℓ with Δ. Since we need to account for shear, we shall no longer use equation (60) but the more general equation (35f), where we shall write (Rodi 1984; Hossain & Rodi 1982)

$$-\overline{u_i u_j} \frac{\partial U_i}{\partial x_j} = \nu_t S^2 , \qquad S^2 = \frac{1}{2} \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right)^2 , \tag{90}$$

so that finally

$$\epsilon = \nu_t S^2 + \kappa_t N^2 . \tag{91}$$

In analogy with equation (89), one writes

$$\nu_t = \ell_\nu e^{1/2} , \qquad \ell_\nu = c_\nu \Delta , \qquad \pi^2 c_\nu = c_\epsilon , \tag{92}$$

where c_ϵ is given by equation (73b). Rewriting equation (91) as

$$\epsilon = \nu_t S^2 (1 + \sigma_t^{-1} \mathrm{Ri}) , \tag{93}$$

where σ_t is the turbulent Prandtl number ν_t/κ_t, using equation (73a) we get an expression for the energy e. Substituting the result into equation (92), we obtain, with $C_*^2 = c_\nu^3 c_\epsilon^{-1}$,

$$\nu_t = C_* \Delta^2 S \left(1 + \frac{1}{\sigma_t} \mathrm{Ri} \right)^{1/2} , \tag{94}$$

which is the expression first suggested by Lilly (1962) and used recently by Eidson (1985). While equation (94) is evidently formally correct, the problem is to compute the turbulent Prandtl number σ_t, which in principle is not a constant but a function of Ri.

To that end, making use of equation (73a), we obtain from equations (91) and (92)

$$c_\epsilon e = \Delta S^2 (c_\nu \Delta + \ell_t \mathrm{Ri}) . \tag{95}$$

Next, we substitute ℓ_t from equation (89). The resulting expression for e is then used to obtain

$$\nu_t = c_\nu \Delta^2 S [X + (X^2 - A_2 \pi^{-2} \mathrm{Ri})^{1/2}]^{1/2} , \tag{96}$$

$$\kappa_t = \nu_t (A_1/c_\nu)(1 - A_2 c_\nu^2 N^2 \Delta^4 \nu_t^{-2})^{-1} , \tag{97}$$

where we have defined

$$2\pi^2 X = 1 + \pi^2 A_3 \mathrm{Ri} . \tag{98}$$

Therefore, the turbulent Prandtl number is indeed not constant but

$$\sigma_t(N) = \sigma_t(0)(1 - A_2 c_\nu^2 N^2 \Delta^4 \nu_t^{-2}) , \tag{99}$$

where $\sigma_t(0) = c_\nu/A_1 =$ constant.

Equations (90)–(92) are the expressions for the turbulent viscosity and turbulent conductivity that replace Smagorinsky's formula (87) in the presence of buoyancy and at the same time generalize Lilly's formula (94). Using the new formula for ν_t, Fox & Sofia (1991) have obtained preliminary results which indicate an overall improvement.

Finally, equations (90)–(92) could also be used in the study of accretion disks in lieu of the empirical formula (Pringle 1981; Rudiger 1987),

$$\nu_t = \alpha c_s H , \tag{100}$$

where α is a free parameter, c_s is the sound speed, and H is the height of the disk.

We must express a word of caution about equations (96)–(97). In fact, we feel that while equation (96) certainly improves the Smagorinsky's expression (87), it probably still underestimates the true value of ν_t. The suspicion is borne out by the fact that we have assumed that ℓ_ν in equation (92) is a constant, while comparison with equation (89) indicates that the corresponding ℓ_t is actually larger than Δ due to the presence of the buoyancy term N^2 in the denominator. A quantitative analysis of this effect requires a more complex study than the one that led us to equation (96), which we suggest ought to be viewed as a first-order correction to Smagorinsky's formula.

16. CONCLUSIONS

Turbulent convection is such a complex physical phenomenon that no model is capable of accounting for all its important features. The advent of the MLT, which suggested equation (13), offered a way to calculate bulk properties *only*, and as such the MLT has demonstrably been a useful guide. It can be improved, as recent work has shown (CM1, 2; Chan & Sofia 1989).

There is, however, a phenomenon that has eluded the MLT: *overshooting*, Worse yet, treatments using the MLT have given rise to such contrasting results that the reality of the phenomenon itself has been doubted. Geophysical, numerical simulations and laboratory data have dispelled such doubts (Zahn 1991). The phenomenon is important and must therefore be quantified (Marcus et al. 1983; Andersen et al. 1990; Stothers & Chin 1991).

With the wisdom of hindsight, one can say that the MLT is inadequate to treat overshooting because it is based on the assumption that convection is homogeneous throughout the convective zone, while overshooting is a manifestation of inhomogeneity. The MLT was not constructed to deal with overshooting but as a total to compute bulk properties which are ostensibly less sensitive to the inhomogeneity assumption. One cannot therefore fault the MLT if the overshooting problem is in a poor state. The MLT was devised to handle a specific task, and extrapolations to phenomena for which it was not tailored are bound to be unsuccessful at best and misleading at worst.

In this paper we suggest the use of the Reynolds stress formalism which yields all the turbulent quantities of interest and which incorporates overshooting. Effects due to rotation can also be included.

The complete model consists of differential equations for $\overline{w\theta}$, $\overline{w^2}$, $\overline{q^2}$, $\overline{\theta^2}$, ϵ, *and* ϵ_θ. *The flux conservation law is included in the solution of the problem, which therefore also yields the mean temperature profile once the structure of the source, represented by* β_0, *is prescribed.*

The Reynolds stress model departs from the models that have often been used to treat stellar convection. This in itself is of course no guarantee of success; the model contains its own approximations, but at least it strives to include the physical features that are indispensable to understand and qualify overshooting.

The past success of the Reynolds stress model to study atmospheric turbulence, where the presence of both convection and mean flow are even more demanding, seems to bode well for the performance of the model in the case of stellar convection. A final judgment will have to be postponed until the model is actually solved and applied to specific astrophysical cases like accretion disks and stellar interiors.

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APPENDIX A

In a steady state situation, the equations governing the third-order moments can be inverted so as to express the results in the following general form ($\chi = 0$):

$$\begin{aligned} \overline{w\theta^2} &= A_1 \frac{\partial}{\partial z} \overline{w\theta} + A_2 \frac{\partial}{\partial z} \overline{w^2} + A_3 \frac{\partial}{\partial z} \overline{\theta^2} , \\ \overline{w^2\theta} &= B_1 \frac{\partial}{\partial z} \overline{w\theta} + B_2 \frac{\partial}{\partial z} \overline{w^2} + B_3 \frac{\partial}{\partial z} \overline{\theta^2} , \\ \overline{w^3} &= C_1 \frac{\partial}{\partial z} \overline{w\theta} + C_2 \frac{\partial}{\partial z} \overline{w^2} + C_3 \frac{\partial}{\partial z} \overline{\theta^2} . \end{aligned} \tag{A1}$$

It should be noticed that with the down-gradient approximation (eq. [36]) we would have

$$\begin{aligned} A_1 &= A_2 = 0 , \\ B_2 &= B_3 = 0 , \\ C_1 &= C_3 = 0 . \end{aligned} \tag{A2}$$

Moreover, the "eddy-viscosity" coefficients A, B, and C have the following general structure:

$$a_1 \tau \overline{w^2} + a_2 g\alpha\tau^2 \overline{w\theta} \tag{A3}$$

where one clearly sees that buoyancy plays a basic role that a simple relation like equation (9) is unable to account for.

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